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Quantitative comparison between theoretical predictions and experimental results for Bragg spectroscopy of a strongly interacting Fermi superfluid

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Theoretical predictions for the dynamic structure factor of a harmonically trapped Fermi superfluid near the Bose-Einstein condensate–Bardeen-Cooper-Schrieffer (BEC-BCS) crossover are compared with recent Bragg spectroscopy measurements at large transferred momenta. The calculations are based on a random-phase (or time-dependent Hartree-Fock-Gorkov) approximation generalized to the strongly interacting regime. Excellent agreement with experimental spectra at low temperatures is obtained, with no free parameters. Theoretical predictions for zero-temperature static structure factor are also found to agree well with the experimental results and independent theoretical calculations based on the exact Tan relations. The temperature dependence of the structure factors at unitarity is predicted.

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Ultracold Fermi gases of ^{6}Li and ^{40}K atoms near Feshbach resonances provide a new paradigm for studying strongly correlated many-body systems [1]. At low temperatures, they display the intriguing crossover from a Bose-Einstein condensate (BEC) to a Bardeen-Cooper-Schrieffer (BCS) superfluid [2]. In the unitarity regime at the cusp of the crossover, a superfluid with neither dominant bosonic nor fermionic character emerges that exhibits universal properties that might be found in other strongly interacting superfluids [3,4], such as high-temperature superconductors or nuclear matter in neutron stars. This new superfluid has already been investigated intensively [1,2], leading to several milestone observations, some of which still defy theoretical understanding. Here we present a quantitative description of the recent two-photon Bragg spectroscopy measurement for this new superfluid [5].

Theoretical challenges in describing the BEC-BCS crossover arise from its strongly correlated nature: there is no small interaction parameter to set the accuracy of theories [6]. Significant progress has been made in developing better quantum Monte Carlo simulations [7–10] and strong-coupling theories [6,11–14], leading to the quantitative establishment of a number of properties. These include equation of state [6,7,12,15–17], frequency of collective oscillations [18,19], pairing gap [10,20], and superfluid transition temperature [9,21]. However, other fundamental properties, such as the single-particle spectral function measured by rf spectroscopy [22,23] and the dynamic structure factor probed by Bragg spectroscopy [5], are not as well understood.

In this Rapid Communication, we show that a random-phase approximation (RPA), generalized to the strongly interacting regime, is able to describe quantitatively the observed Bragg spectra for harmonically trapped ^{6}Li atoms at large transferred momenta. This surprising result indicates that the RPA captures the essential physics and constitutes a reasonable approximation for the strongly interacting region of the BEC-BCS crossover, particularly the low temperature range accessed by most experiments. The RPA method has previously been used to study the dynamic structure factor [24] and collective oscillations [25] of weakly interacting Fermi superfluids. A dynamic mean-field approach, identical to the RPA but based on kinetic equations, was developed to investigate structure factors [26] and collective modes [27] of a uniform, strongly interacting Fermi gas. At finite temperatures, structure factors at the crossover were also studied using a pseudogap theory [28].

Our main result is summarized in Fig. 1, which shows the normalized experimental Bragg spectra [5] along with the RPA predictions. Excellent agreement is found, with no free parameters.

We begin by outlining briefly the RPA using the Hamiltonian (hereafter $\hbar = 1$),

$$\mathcal{H} = \sum_\sigma \int d\mathbf{r}\psi_\sigma^+(\mathbf{r})\left[-\frac{\nabla^2}{2M} - \mu + V_T(\mathbf{r})\right]\psi_\sigma(\mathbf{r}) + U_0 \int d\mathbf{r}\psi_\uparrow^+(\mathbf{r})\psi_\downarrow^+(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}), \quad (1)$$

which describes a balanced spin-1/2 ($\sigma = \uparrow,\downarrow$) Fermi gas with mass M in a harmonic trap $V_T(\mathbf{r})$, where fermions with unlike spins interact via a contact potential $U_0\delta(\mathbf{r}-\mathbf{r}')$. The total number of atoms N is tuned by the chemical potential μ and the bare interaction strength U_0 is renormalized by the s-wave scattering length a, $1/U_0 + \sum_{\mathbf{k}} M/\mathbf{k}^2 = M/(4\pi a)$. In the superfluid phase, we treat the system as a gas of long-lived Bogoliubov quasiparticles interacting through a mean-field and consider its response to a weak external field of the form of $\delta V e^{i(\mathbf{qr}-\omega t)}$. The essential idea of the RPA is that there is a self-generated mean-field potential experienced by quasiparticles [29], associated with the local changes in the density distribution of the two spin species, $\delta U = U_0 \int d\mathbf{r}(\sum_\sigma \delta n_\sigma \psi_\sigma^+\psi_\sigma + \delta m \psi_\uparrow^+\psi_\downarrow^+ + \delta m^*\psi_\downarrow\psi_\uparrow)$, where $\delta n_\sigma \equiv \delta n_\sigma(\mathbf{r},t)$ and $\delta m \equiv \delta m(\mathbf{r},t)$ are the normal and anomalous density fluctuations, respectively, which must be determined self-consistently. In the linear approximation, the self-generated potential δU plays the same role as the perturbation field when we calculate

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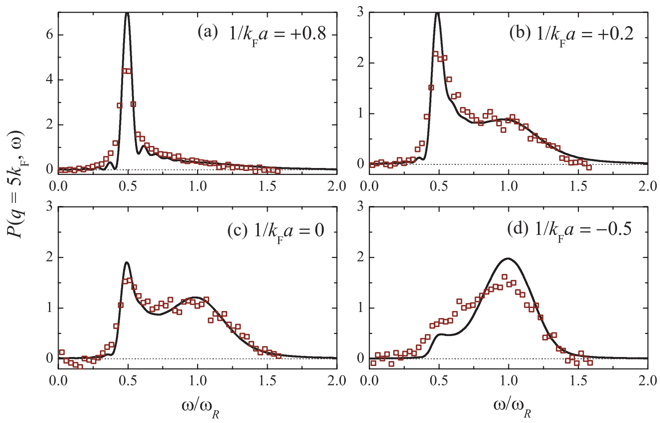

FIG. 1. (Color online) Quantitative comparison of theoretical and experimental Bragg spectra [see Eq. (6)]. The RPA prediction (lines) agrees well with the experimental data (empty squares) [5] at the BEC-BCS crossover, with no free parameters. The spectrum is normalized so that the area below the curve is unity. The frequency is measured in units of the recoil energy of the atoms (see text).

the dynamic response using a static BCS Hamiltonian as the reference system [24,25,29]. This leads to coupled equations for density fluctuations. The linear response is characterized by a matrix consisting of all two-particle response functions:

$$\chi \equiv \begin{Bmatrix} \langle\langle \hat{n}_\uparrow \hat{n}_\uparrow \rangle\rangle & \langle\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle\rangle & \langle\langle \hat{n}_\uparrow \hat{m} \rangle\rangle & \langle\langle \hat{n}_\uparrow \hat{m}^+ \rangle\rangle \\ \langle\langle \hat{n}_\downarrow \hat{n}_\uparrow \rangle\rangle & \langle\langle \hat{n}_\downarrow \hat{n}_\downarrow \rangle\rangle & \langle\langle \hat{n}_\downarrow \hat{m} \rangle\rangle & \langle\langle \hat{n}_\downarrow \hat{m}^+ \rangle\rangle \\ \langle\langle \hat{m} \hat{n}_\uparrow \rangle\rangle & \langle\langle \hat{m} \hat{n}_\downarrow \rangle\rangle & \langle\langle \hat{m} \hat{m} \rangle\rangle & \langle\langle \hat{m} \hat{m}^+ \rangle\rangle \\ \langle\langle \hat{m}^+ \hat{n}_\uparrow \rangle\rangle & \langle\langle \hat{m}^+ \hat{n}_\downarrow \rangle\rangle & \langle\langle \hat{m}^+ \hat{m} \rangle\rangle & \langle\langle \hat{m}^+ \hat{m}^+ \rangle\rangle \end{Bmatrix},$$

where $\langle\langle \hat{A}\hat{B} \rangle\rangle$ is the Fourier transform of the retarded function $-i\Theta\left(t-t'\right)\langle[\hat{A}(\mathbf{r},t),\hat{B}(\mathbf{r}',t')]\rangle$. For simplicity, we abbreviate $\chi_{\sigma\sigma'} \equiv \langle\langle \hat{n}_\sigma \hat{n}_{\sigma'} \rangle\rangle$, $\chi_{\sigma m} \equiv \langle\langle \hat{n}_\sigma \hat{m} \rangle\rangle$, $\chi_{\sigma \bar{m}} \equiv \langle\langle \hat{n}_\sigma \hat{m}^+ \rangle\rangle$, $\chi_{m\bar{m}} \equiv \langle\langle \hat{m}\hat{m}^+ \rangle\rangle$, and so on. By solving the coupled equations for density fluctuations, the standard RPA response function χ can be expressed in terms of the static BCS response function χ^0 [25],

$$\chi = \chi^0[\hat{1} - U_0 \chi^0 \mathcal{G}]^{-1}, \tag{2}$$

where $\mathcal{G} = \delta(\mathbf{r}-\mathbf{r}')[\sigma_0 \otimes \sigma_x]$ is a direct product of two Pauli matrices σ_0 and σ_x and the unit matrix $\hat{1} = \delta(\mathbf{r}-\mathbf{r}')[\sigma_0 \otimes \sigma_0]$. The dynamic structure factor $S_{\sigma\sigma'}(\omega)$ is related to the normal density response function by the fluctuation-dissipation theorem,

$$S_{\sigma\sigma'}(\omega) = -\frac{1}{\pi}\frac{1}{[1-\exp(-\omega/k_B T)]}\,\mathrm{Im}\,\chi_{\sigma\sigma'}(\omega), \tag{3}$$

and the static structure factor is given by $S_{\sigma\sigma'} = (2/N)\int_{-\infty}^{+\infty} d\omega S_{\sigma\sigma'}(\omega)$. In the weak-coupling regime, Eq. (2) can be solved by calculating χ^0 for a thermal average of BCS quasiparticles [24,25].

Here, we extend the RPA to the strongly interacting regime with an arbitrarily large scattering length a, by properly renormalizing the bare interaction strength U_0 and the two response functions $\chi^0_{m\bar{m}}$ and $\chi^0_{\bar{m}m}$, which was found to be suitable at the BEC-BCS crossover [14,30]. The ultraviolet divergence of these two functions [25] is canceled exactly by the small value of U_0, when the momentum cutoff goes to infinity. In homogeneous systems, a careful account of the divergent terms in the inverted matrix of the RPA equation (2) leads to a concise expression for the response functions:

$$\chi_{\uparrow\uparrow} = \chi^0_{\uparrow\uparrow} - \left[2\chi^0_{\uparrow\downarrow}\chi^0_{\uparrow m}\chi^0_{\uparrow\bar{m}} + \left(\chi^0_{\uparrow m}\right)^2 \tilde{\chi}^0_{m\bar{m}} + \left(\chi^0_{\uparrow\bar{m}}\right)^2 \tilde{\chi}^0_{\bar{m}m}\right] \Big/ \left[\tilde{\chi}^0_{m\bar{m}}\tilde{\chi}^0_{\bar{m}m} - \left(\chi^0_{\uparrow\downarrow}\right)^2\right], \tag{4}$$

and

$$\chi_{\uparrow\downarrow} = \chi_{\uparrow\uparrow} - \chi^0_{\uparrow\uparrow} + \chi^0_{\uparrow\downarrow}, \tag{5}$$

where the response functions with a tilde, i.e., $\tilde{\chi}^0_{m\bar{m}} \equiv \chi^0_{m\bar{m}} + \sum_{\mathbf{k}} M/\mathbf{k}^2 - M/(4\pi a)$, become free from any ultraviolet divergence. The above equations were previously obtained by Combescot and collaborators using kinetic equations (see Eq. (B22) in Ref. [27]). Note that, we use a Leggett-BCS ground state without inclusion of the Hartree-Fock term in the quasiparticle spectrum. Therefore, in the BCS regime our treatment does not account for the leading interaction effect as in Refs. [24,25]. At the crossover, however, it does capture the dominant pairing gap. Note also that, the RPA method accounts for single particle-hole excitations. Higher correlations such as multi-particle-hole excitations are neglected.

In the presence of a harmonic trap, the renormalization procedure becomes cumbersome because of the discrete energy levels. It is convenient to use a local density approximation (LDA) that treats the system as a collection of many homogeneous cells with local chemical potential [2], $\mu(\mathbf{r}) = \mu - V_T(\mathbf{r})$, where $V_T(\mathbf{r}) = M(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2$ is the harmonic trapping potential. The LDA treatment is valid for a large number of atoms such as $N \sim 10^5$ as in experiments. It has been used extensively in studying the static density profile of either atomic Fermi, Bose gases [31] or Bose-Fermi mixtures [32]. In the nuclear context, it has also been used to calculate the dynamic response function [33]. At a given temperature and scattering length, we solve the Leggett-BCS equation with local chemical potential for the local pairing gap and calculate the static response function χ^0, then solve the local RPA density response functions using Eqs. (4) and (5), and finally obtain the total RPA responses by integrating over the whole trap. In our calculations, the interaction strength is characterized by the dimensionless parameter, $1/(k_F a)$, where $k_F = \sqrt{2ME_F}$ is the Fermi wave vector and the Fermi energy is $E_F = (3N\omega_x\omega_y\omega_z)^{1/3}$.

Figure 2 shows the zero-temperature spin parallel, antiparallel, and total dynamic structure factor at a transferred wavevector $q = 5k_F$ in the BEC-BCS crossover, calculated using the above RPA procedure for a trapped Fermi gas. In addition to a broad response at the recoil energy $\omega_R = q^2/(2M) = 25E_F$ caused by resonant scattering of atoms, a much narrower peak develops at about $\omega_R/2$ with increased coupling. The peak, commonly referred to as the quasielastic peak in the literature, is found by the recent theoretical calculation [26] and the observation of Bragg spectroscopy [5]. This is simply the Bogoliubov-Anderson phonon mode of a Fermi superfluid at large wave-vectors, which evolves continuously into a Bogoliubov mode of molecules toward the BEC limit [26]. The molecular peak is mostly evident in $S_{\uparrow\downarrow}$ as there is no background atomic response. Measurements of $S_{\uparrow\downarrow}$ may also help establish the presence of Fermi superfluidity [28].

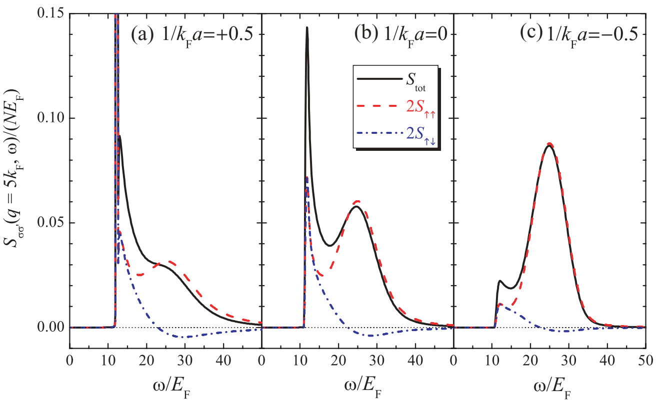

FIG. 2. (Color online) Zero temperature spin parallel $S_{\uparrow\uparrow}(\mathbf{q},\omega)$ (dashed lines), antiparallel $S_{\uparrow\downarrow}(\mathbf{q},\omega)$ (dot-dashed lines), and total dynamic structure factor $S(\mathbf{q},\omega) = 2[S_{\uparrow\uparrow} + S_{\uparrow\downarrow}]$ (solid lines) across the BEC-BCS crossover: $1/k_F a = 0.5$ (a), 0.0 (b), and -0.5 (c). The negative weight in $S_{\uparrow\downarrow}$ at about the recoil energy is consistent with the exact sum rule $\int \omega S_{\uparrow\downarrow}(\mathbf{q},\omega) d\omega = 0$ [28].

To make a quantitative comparison with the experimental spectra, we calculate the momentum imparted to the Fermi cloud, the quantity measured directly in the Bragg scattering experiment [5,34]:

$$\mathcal{P}(\mathbf{q},\omega) \propto \frac{1}{\pi\sigma}\int_{-\infty}^{\infty} d\omega' S(\mathbf{q},\omega')\mathrm{sinc}^2\left[\frac{\omega-\omega'}{\sigma}\right], \qquad (6)$$

where $\mathrm{sinc}(x) = \sin(x)/x$ and the energy resolution $\sigma = 2/\tau_{Br}$ is set by the experimental Bragg pulse duration ($\tau_{Br} = 40\,\mu$s) [5]. We find $\sigma \approx 0.68 E_F \approx 0.027\omega_R$. Figure 1 presents a comparison of the experimental data (open squares) with the RPA predictions (lines) for the Bragg spectra normalized in such a way that $\int \mathcal{P}(\mathbf{q},\omega)d\omega = 1$. With no free parameters, our RPA predictions agree well with the experimental results in the unitarity regime ($1/k_F a = 0.0$ and 0.2) and BEC regime ($1/k_F a = 0.8$). The agreement on the BCS side ($1/k_F a = -0.5$), however, becomes worse. The quantitative agreement around unitarity is very compelling, since the RPA was assumed to be unreliable in the (strongly interacting) regime of large pair fluctuations. Our comparison indicates that the RPA is able to describe the dynamical properties of the BEC-BCS crossover, at least at zero temperature and large momenta. High order multi-particle-hole excitations, absent in the RPA theory, seems to be negligibly small at large momenta. More studies are needed to understand this. Note finally that, the somewhat poorer agreement at $1/k_F a = -0.5$ can be attributed to the mean-field shift, which is ignored in the RPA but dominates for sufficiently weak interactions.

The agreement between the RPA theory and the Bragg experiment is further confirmed by comparing the spin antiparallel static structure factor at zero temperature, as reported in Fig. 3. Experimentally, the static structure factor can be measured model-independently by invoking the f-sum rule [35]; while, theoretically, it can be determined very accurately using the exact Tan relations and the known equation of state [36]. It is evident from Fig. 3 that the RPA prediction fits very well with the experimental data, as well as the independent theoretical result based on the Tan relations. In particular, the two theoretical predictions are nearly indistinguishable on the

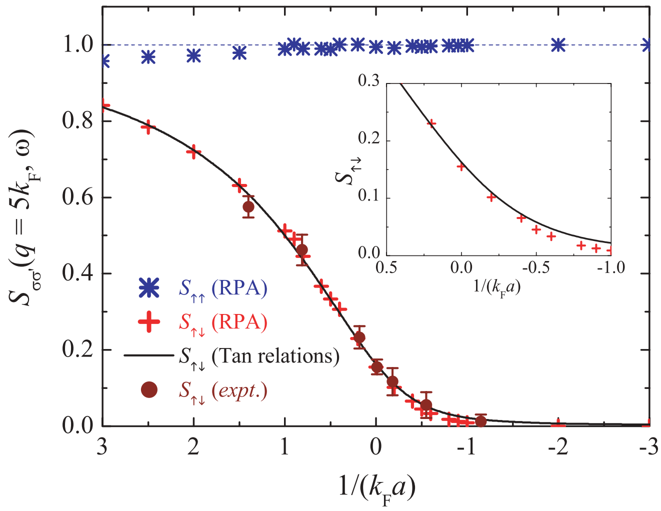

FIG. 3. (Color online) Quantitative comparison between theory and experiment for the zero temperature static structure factor across the crossover. For $S_{\uparrow\downarrow}$, with no free parameters our RPA prediction (plus symbols) agrees well with the experimental data for $S(\mathbf{q},\omega) - 1$ (solid circles with error bars) [35] and an independent theoretical result based on the exact Tan relations (solid line) [36]. At large transferred momentum, $S_{\uparrow\uparrow} \simeq 1$. The inset highlights the RPA prediction with respect to the Tan-relation result in the BCS regime.

BEC side with $1/k_F a \geqslant 0$. However, they differ toward the BCS limit, as highlighted in the inset. The discrepancy is consistent with Fig. 1(d) where the RPA predicts less pairing and hence lower $S(q)$.

A more stringent test of the RPA theory may be provided by the temperature or momentum dependence of dynamic and static structure factors. In Fig. 4, we predict the dynamic and static structure factor as a function of temperature for a trapped Fermi gas at unitarity, which will be investigated in

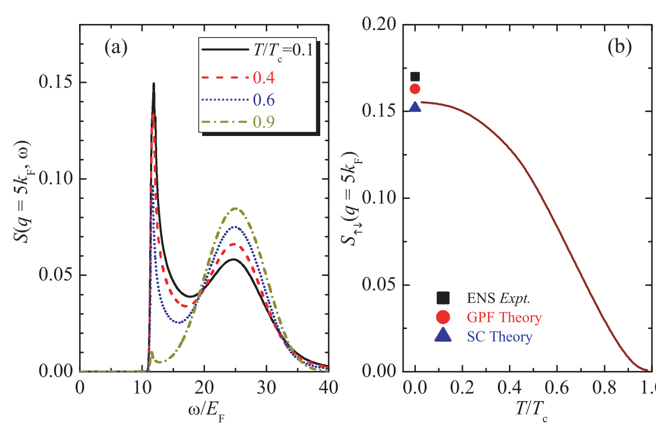

FIG. 4. (Color online) Temperature dependence of the dynamic (a) and static (b) structure factor for a unitary Fermi gas in harmonic traps at $q = 5k_F$. According to the Tan relation, $S_{\uparrow\downarrow}(\mathbf{q}) \simeq 128\zeta/[175\xi^{1/4}(q/k_F)]$ at $T = 0$ [35], where ξ and ζ are the universal parameters at unitarity [17]. The symbols in (b) show predictions using theoretically or experimentally determined ξ and ζ : ENS experiment (square) [17], Gaussian pair fluctuation theory (circle) [12], and self-consistent theory (triangle) [37]. Here, $T_c \simeq 0.37 T_F = 0.37 E_F/k_B$.

future experiments. As anticipated, the pair (atomic) response increases (decreases) with decreasing the temperature, leading to a monotonic decay of the static structure factor.

The present RPA theory is most likely valid only in a narrow temperature window near $T = 0$. With increasing temperature, the pairing gap decreases and thermal pair fluctuations increase. The RPA will eventually break down at a characteristic temperature $T_{RPA}(\lesssim T_c)$. This is evident in Fig. 4(b) where the spin antiparallel static structure factor vanishes unphysically above the superfluid transition temperature.

At low transferred momenta, quantum fluctuations are likely to increase and the RPA theory will become less reliable. To overcome these limitations, we could use a Cooperon-mediated interaction (many-body T-matrix) to replace the bare contact interaction [38], or use the phenomenological Landau parameters for the mean-field shift [39], as determined from thermodynamic measurements [16] or quantum Monte Carlo simulations.

In summary, we have used a strong-coupling RPA theory to calculate the dynamic and static structure factors of a trapped Fermi gas at the BEC-BCS crossover. The theory is quantitatively applicable at low temperatures and large transferred momenta, as confirmed by the excellent agreement with the experimental Bragg spectra. The RPA theory thus seems to provide a novel starting point for investigating dynamic properties of a strongly interacting Fermi gas at finite temperatures and low momenta.

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